APPENDIX B

TOXIC SUBSTANCES

APPENDIX B TOXIC SUBSTANCES

B.1 Data for Toxic Substances

The exhibits in this section of Appendix B provide the data needed to carry out the calculations for regulated toxic substances using the methods presented in the text of this guidance. Exhibit B-1 presents data for toxic gases, Exhibit B-2 presents data for toxic liquids, and Exhibit B-3 presents data for several toxic substances commonly found in water solution and for oleum. Exhibit B-4 provides temperature correction factors that can be used to correct the release rates estimated for pool evaporation of toxic liquids that are released at temperatures between 25 ºC to 50 ºC.

The derivation of the factors presented in Exhibits B-1 - B-4 is discussed in Appendix D. The data used to develop the factors in Exhibits B-1 and B-2 are primarily from Design Institute for Physical Property Data (DIPPR), American Institute of Chemical Engineers, *Physical and Thermodynamic Properties of Pure Chemicals, Data Compilation*. Other sources, including the National Library of Medicine's Hazardous Substances Databank (HSDB) and the *Kirk-Othmer Encyclopedia of Chemical Technology*, were used for Exhibits B-1 and B-2 if data were not available from the DIPPR compilation. The factors in Exhibit B-3 were developed using data primarily from *Perry's Chemical Engineers' Handbook* and the *Kirk-Othmer Encyclopedia of Chemical Technology*. The temperature correction factors in Exhibit B-4 were developed using vapor pressure data derived from the vapor pressure coefficients in the DIPPR compilation.

Exhibit B-1
Data for Toxic Gases

CAS Number	Chemical Name	Molecular Weight	Ratio of Specific Heats	Toxic Endpoint[a]			Liquid Factor Boiling (LFB)	Density Factor (DF) (Boiling)	Gas Factor (GF)[k]	Vapor Pressure @25 °C (psia)	Reference Table[b]
				mg/L	ppm	Basis					
7664-41-7	Ammonia (anhydrous)[c]	17.03	1.31	0.14	200	ERPG-2	0.073	0.71	14	145	Buoyant[d]
7784-42-1	Arsine	77.95	1.28	0.0019	0.6	EHS-LOC (IDLH)	0.23	0.30	30	239	Dense
10294-34-5	Boron trichloride	117.17	1.15	0.010	2	EHS-LOC (Tox[e])	0.22	0.36	36	22.7	Dense
7637-07-2	Boron trifluoride	67.81	1.20	0.028	10	EHS-LOC (IDLH)	0.25	0.31	28	[f]	Dense
7782-50-5	Chlorine	70.91	1.32	0.0087	3	ERPG-2	0.19	0.31	29	113	Dense
10049-04-4	Chlorine dioxide	67.45	1.25	0.0028	1	EHS-LOC equivalent (IDLH)[g]	0.15	0.30	28	24.3	Dense
506-77-4	Cyanogen chloride	61.47	1.22	0.030	12	EHS-LOC equivalent (Tox)[h]	0.14	0.41	26	23.7	Dense
19287-45-7	Diborane	27.67	1.17	0.0011	1	ERPG-2	0.13	1.13	17	[f]	Buoyant[d]
75-21-8	Ethylene oxide	44.05	1.21	0.090	50	ERPG-2	0.12	0.55	22	25.4	Dense
7782-41-4	Fluorine	38.00	1.36	0.0039	2.5	EHS-LOC (IDLH)	0.35	0.32	22	[f]	Dense
50-00-0	Formaldehyde (anhydrous)[c]	30.03	1.31	0.012	10	ERPG-2	0.10	0.59	19	75.2	Dense
74-90-8	Hydrocyanic acid	27.03	1.30	0.011	10	ERPG-2	0.079	0.72	18	14.8	Buoyant[d]
7647-01-0	Hydrogen chloride (anhydrous)[c]	36.46	1.40	0.030	20	ERPG-2	0.15	0.41	21	684	Dense
7664-39-3	Hydrogen fluoride (anhydrous)[c]	20.01	1.40	0.016	20	ERPG-2	0.066	0.51	16	17.7	Buoyant[i]
7783-07-5	Hydrogen selenide	80.98	1.32	0.00066	0.2	EHS-LOC (IDLH)	0.21	0.25	31	151	Dense
7783-06-4	Hydrogen sulfide	34.08	1.32	0.042	30	ERPG-2	0.13	0.51	20	302	Dense
74-87-3	Methyl chloride	50.49	1.26	0.82	400	ERPG-2	0.14	0.48	24	83.2	Dense
74-93-1	Methyl mercaptan	48.11	1.20	0.049	25	ERPG-2	0.12	0.55	23	29.2	Dense
10102-43-9	Nitric oxide	30.01	1.38	0.031	25	EHS-LOC (TLV[j])	0.21	0.38	19	[f]	Dense
75-44-5	Phosgene	98.92	1.17	0.00081	0.2	ERPG-2	0.20	0.35	33	27.4	Dense

Exhibit B-1 (continued)

CAS Number	Chemical Name	Molecular Weight	Ratio of Specific Heats	Toxic Endpoint[a]			Liquid Factor Boiling (LFB)	Density Factor (DF) (Boiling)	Gas Factor (GF)[k]	Vapor Pressure @25 °C (psia)	Reference Table[b]
				mg/L	ppm	Basis					
7803-51-2	Phosphine	34.00	1.29	0.0035	2.5	ERPG-2	0.15	0.66	20	567	Dense
7446-09-5	Sulfur dioxide (anhydrous)	64.07	1.26	0.0078	3	ERPG-2	0.16	0.33	27	58.0	Dense
7783-60-0	Sulfur tetrafluoride	108.06	1.30	0.0092	2	EHS-LOC (Tox[e])	0.25	0.25 (at -73 °C)	36	293	Dense

Notes:

[a] Toxic endpoints are specified in Appendix A to 40 CFR part 68 in units of mg/L. To convert from units of mg/L to mg/m^3, multiply by 1,000. To convert mg/L to ppm, use the following equation:

$$Endpoint_{ppm} = \frac{Endpoint_{mg/L} \times 1{,}000 \times 24.5}{Molecular\ Weight}$$

[b] "Buoyant" in the Reference Table column refers to the tables for neutrally buoyant gases and vapors; "Dense" refers to the tables for dense gases and vapors. See Appendix D, Section D.4.4, for more information on the choice of reference tables.
[c] See Exhibit B-3 of this appendix for data on water solutions.
[d] Gases that are lighter than air may behave as dense gases upon release if liquefied under pressure or cold; consider the conditions of release when choosing the appropriate table.
[e] LOC is based on the IDLH-equivalent level estimated from toxicity data.
[f] Cannot be liquefied at 25 °C.
[g] Not an EHS; LOC-equivalent value was estimated from one-tenth of the IDLH.
[h] Not an EHS; LOC-equivalent value was estimated from one-tenth of the IDLH-equivalent level estimated from toxicity data.
[i] Hydrogen fluoride is lighter than air, but may behave as a dense gas upon release under some circumstances (e.g., release under pressure, high concentration in the released cloud) because of hydrogen bonding; consider the conditions of release when choosing the appropriate table.
[j] LOC based on Threshold Limit Value (TLV) - Time-weighted average (TWA) developed by the American Conference of Governmental Industrial Hygienists (ACGIH).
[k] Use GF for gas leaks under choked (maximum) flow conditions.

Exhibit B-2
Data for Toxic Liquids

CAS Number	Chemical Name	Molecular Weight	Vapor Pressure at 25 °C (mm Hg)	Toxic Endpoint[a]			Liquid Factors		Density Factor (DF)	Liquid Leak Factor (LLF)[I]	Reference Table[b]	
				mg/L	ppm	Basis	Ambient (LFA)	Boiling (LFB)			Worst Case	Alternative Case
107-02-8	Acrolein	56.06	274	0.0011	0.5	ERPG-2	0.047	0.12	0.58	40	Dense	Dense
107-13-1	Acrylonitrile	53.06	108	0.076	35	ERPG-2	0.018	0.11	0.61	39	Dense	Dense
814-68-6	Acrylyl chloride	90.51	110	0.00090	0.2	EHS-LOC (Tox[c])	0.026	0.15	0.44	54	Dense	Dense
107-18-6	Allyl alcohol	58.08	26.1	0.036	15	EHS-LOC (IDLH)	0.0046	0.11	0.58	41	Dense	Buoyant[d]
107-11-9	Allylamine	57.10	242	0.0032	1	EHS-LOC (Tox[c])	0.042	0.12	0.64	36	Dense	Dense
7784-34-1	Arsenous trichloride	181.28	10	0.01	1	EHS-LOC (Tox[c])	0.0037	0.21	0.23	100	Dense	Buoyant[d]
353-42-4	Boron trifluoride compound with methyl ether (1:1)	113.89	11	0.023	5	EHS-LOC (Tox[c])	0.0030	0.16	0.49	48	Dense	Buoyant[d]
7726-95-6	Bromine	159.81	212	0.0065	1	ERPG-2	0.073	0.23	0.16	150	Dense	Dense
75-15-0	Carbon disulfide	76.14	359	0.16	50	ERPG-2	0.075	0.15	0.39	60	Dense	Dense
67-66-3	Chloroform	119.38	196	0.49	100	EHS-LOC (IDLH)	0.055	0.19	0.33	71	Dense	Dense
542-88-1	Chloromethyl ether	114.96	29.4	0.00025	0.05	EHS-LOC (Tox[c])	0.0080	0.17	0.37	63	Dense	Dense
107-30-2	Chloromethyl methyl ether	80.51	199	0.0018	0.6	EHS-LOC (Tox[c])	0.043	0.15	0.46	51	Dense	Dense
4170-30-3	Crotonaldehyde	70.09	33.1	0.029	10	ERPG-2	0.0066	0.12	0.58	41	Dense	Buoyant[d]
123-73-9	Crotonaldehyde, (E)-	70.09	33.1	0.029	10	ERPG-2	0.0066	0.12	0.58	41	Dense	Buoyant[d]
108-91-8	Cyclohexylamine	99.18	10.1	0.16	39	EHS-LOC (Tox[c])	0.0025	0.14	0.56	41	Dense	Buoyant[d]
75-78-5	Dimethyldichlorosilane	129.06	141	0.026	5	ERPG-2	0.042	0.20	0.46	51	Dense	Dense
57-14-7	1,1-Dimethylhydrazine	60.10	157	0.012	5	EHS-LOC (IDLH)	0.028	0.12	0.62	38	Dense	Dense
106-89-8	Epichlorohydrin	92.53	17.0	0.076	20	ERPG-2	0.0040	0.14	0.42	57	Dense	Buoyant[d]
107-15-3	Ethylenediamine	60.10	12.2	0.49	200	EHS-LOC (IDLH)	0.0022	0.13	0.54	43	Dense	Buoyant[d]
151-56-4	Ethyleneimine	43.07	211	0.018	10	EHS-LOC (IDLH)	0.030	0.10	0.58	40	Dense	Dense
110-00-9	Furan	68.08	600	0.0012	0.4	EHS-LOC (Tox[c])	0.12	0.14	0.52	45	Dense	Dense
302-01-2	Hydrazine	32.05	14.4	0.011	8	EHS-LOC (IDLH)	0.0017	0.069	0.48	48	Buoyant[d]	Buoyant[d]

Exhibit B-2 (continued)

CAS Number	Chemical Name	Molecular Weight	Vapor Pressure at 25 °C (mm Hg)	Toxic Endpoint[a]			Liquid Factors		Density Factor (DF)	Liquid Leak Factor (LLF)[I]	Reference Table[b]	
				mg/L	ppm	Basis	Ambient (LFA)	Boiling (LFB)			Worst Case	Alternative Case
13463-40-6	Iron, pentacarbonyl-	195.90	40	0.00044	0.05	EHS-LOC (Tox[c])	0.016	0.24	0.33	70	Dense	Dense
78-82-0	Isobutyronitrile	69.11	32.7	0.14	50	ERPG-2	0.0064	0.12	0.63	37	Dense	Buoyant[d]
108-23-6	Isopropyl chloroformate	122.55	28	0.10	20	EHS-LOC (Tox[c])	0.0080	0.17	0.45	52	Dense	Dense
126-98-7	Methacrylonitrile	67.09	71.2	0.0027	1	EHS-LOC (TLV[e])	0.014	0.12	0.61	38	Dense	Dense
79-22-1	Methyl chloroformate	94.50	108	0.0019	0.5	EHS-LOC (Tox[c])	0.026	0.16	0.40	58	Dense	Dense
60-34-4	Methyl hydrazine	46.07	49.6	0.0094	5	EHS-LOC (IDLH)	0.0074	0.094	0.56	42	Dense	Buoyant[d]
624-83-9	Methyl isocyanate	57.05	457	0.0012	0.5	ERPG-2	0.079	0.13	0.52	45	Dense	Dense
556-64-9	Methyl thiocyanate	73.12	10	0.085	29	EHS-LOC (Tox[c])	0.0020	0.11	0.45	51	Dense	Buoyant[d]
75-79-6	Methyltrichlorosilane	149.48	173	0.018	3	ERPG-2	0.057	0.22	0.38	61	Dense	Dense
13463-39-3	Nickel carbonyl	170.73	400	0.00067	0.1	EHS-LOC (Tox[c])	0.14	0.26	0.37	63	Dense	Dense
7697-37-2	Nitric acid (100%)[f]	63.01	63.0	0.026	10	EHS-LOC (Tox[c])	0.012	0.12	0.32	73	Dense	Dense
79-21-0	Peracetic acid	76.05	13.9	0.0045	1.5	EHS-LOC (Tox[c])	0.0029	0.12	0.40	58	Dense	Buoyant[d]
594-42-3	Perchloromethylmercaptan	185.87	6	0.0076	1	EHS-LOC (IDLH)	0.0023	0.20	0.29	81	Dense	Buoyant[d]
10025-87-3	Phosphorus oxychloride	153.33	35.8	0.0030	0.5	EHS-LOC (Tox[c])	0.012	0.20	0.29	80	Dense	Dense
7719-12-2	Phosphorus trichloride	137.33	120	0.028	5	EHS-LOC (IDLH)	0.037	0.20	0.31	75	Dense	Dense
110-89-4	Piperidine	85.15	32.1	0.022	6	EHS-LOC (Tox[c])	0.0072	0.13	0.57	41	Dense	Buoyant[d]
107-12-0	Propionitrile	55.08	47.3	0.0037	1.6	EHS-LOC (Tox[c])	0.0080	0.10	0.63	37	Dense	Buoyant[d]
109-61-5	Propyl chloroformate	122.56	20.0	0.010	2	EHS-LOC (Tox[c])	0.0058	0.17	0.45	52	Dense	Buoyant[d]
75-55-8	Propyleneimine	57.10	187	0.12	50	EHS-LOC (IDLH)	0.032	0.12	0.61	39	Dense	Dense
75-56-9	Propylene oxide	58.08	533	0.59	250	ERPG-2	0.093	0.13	0.59	40	Dense	Dense
7446-11-9	Sulfur trioxide	80.06	263	0.010	3	ERPG-2	0.057	0.15	0.26	91	Dense	Dense
75-74-1	Tetramethyllead	267.33	22.5	0.0040	0.4	EHS-LOC (IDLH)	0.011	0.29	0.24	96	Dense	Dense
509-14-8	Tetranitromethane	196.04	11.4	0.0040	0.5	EHS-LOC (IDLH)	0.0045	0.22	0.30	78	Dense	Buoyant[d]

Exhibit B-2 (continued)

CAS Number	Chemical Name	Molecular Weight	Vapor Pressure at 25 °C (mm Hg)	Toxic Endpoint[a]			Liquid Factors		Density Factor (DF)	Liquid Leak Factor (LLF)[I]	Reference Table[b]	
				mg/L	ppm	Basis	Ambient (LFA)	Boiling (LFB)			Worst Case	Alternative Case
7550-45-0	Titanium tetrachloride	189.69	12.4	0.020	2.6	ERPG-2	0.0048	0.21	0.28	82	Dense	Buoyant[d]
584-84-9	Toluene 2,4-diisocyanate	174.16	0.017	0.0070	1	EHS-LOC (IDLH)	0.000006	0.16	0.40	59	Buoyant[d]	Buoyant[d]
91-08-7	Toluene 2,6-diisocyanate	174.16	0.05	0.0070	1	EHS-LOC (IDLH[g])	0.000018	0.16	0.40	59	Buoyant[d]	Buoyant[d]
26471-62-5	Toluene diisocyanate (unspecified isomer)	174.16	0.017	0.0070	1	EHS-LOC equivalent (IDLH[h])	0.000006	0.16	0.40	59	Buoyant[d]	Buoyant[d]
75-77-4	Trimethylchlorosilane	108.64	231	0.050	11	EHS-LOC (Tox[c])	0.061	0.18	0.57	41	Dense	Dense
108-05-4	Vinyl acetate monomer	86.09	113	0.26	75	ERPG-2	0.026	0.15	0.53	45	Dense	Dense

Notes:

[a] Toxic endpoints are specified in the Appendix A to 40 CFR part 68 in units of mg/L. To convert from units of mg/L to mg/m^3, multiply by 1,000. To convert mg/L to ppm, use the following equation:

$$Endpoint_{ppm} = \frac{Endpoint_{mg/L} \times 1{,}000 \times 24.5}{Molecular\ Weight}$$

[b] "Buoyant" in the Reference Table column refers to the tables for neutrally buoyant gases and vapors; "Dense" refers to the tables for dense gases and vapors. See Appendix D, Section D.4.4, for more information on the choice of reference tables.

[c] LOC is based on IDLH-equivalent level estimated from toxicity data.

[d] Use dense gas table if substance is at an elevated temperature.

[e] LOC based on Threshold Limit Value (TLV) - Time-weighted average (TWA) developed by the American Conference of Governmental Industrial Hygienists (ACGIH).

[f] See Exhibit B-3 of this appendix for data on water solutions.

[g] LOC for this isomer is based on IDLH for toluene 2,4-diisocyanate.

[h] Not an EHS; LOC-equivalent value is based on IDLH for toluene 2,4-diisocyanate.

[i] Use the LLF only for leaks from tanks at atmospheric pressure.

Exhibit B-3
Data for Water Solutions of Toxic Substances and for Oleum
For Wind Speeds of 1.5 and 3.0 Meters per Second (m/s)

CAS Number	Regulated Substance in Solution	Molecular Weight	Toxic Endpoint[a]			Initial Concentration (Wt %)	10-min. Average Vapor Pressure (mm Hg)		Liquid Factor at 25° C (LFA)		Density Factor (DF)	Liquid Leak Factor (LLF)	Reference Table[b]	
			mg/L	ppm	Basis		1.5 m/s	3.0 m/s	1.5 m/s	3.0 m/s			Worst	Alternative
7664-41-7	Ammonia	17.03	0.14	200	ERPG-2	30	332	248	0.026	0.019	0.55	43	Buoyant	Buoyant
						24	241	184	0.019	0.014	0.54	44	Buoyant	Buoyant
						20	190	148	0.015	0.011	0.53	44	Buoyant	Buoyant
50-00-0	Formaldehyde	30.027	0.012	10	ERPG-2	37	1.5	1.4	0.0002	0.0002	0.44	53	Buoyant	Buoyant
7647-01-0	Hydrochloric acid	36.46	0.030	20	ERPG-2	38	78	55	0.010	0.0070	0.41	57	Dense	Buoyant [d]
						37	67	48	0.0085	0.0062	0.42	57	Dense	Buoyant [d]
						36[c]	56	42	0.0072	0.0053	0.42	57	Dense	Buoyant [d]
						34[c]	38	29	0.0048	0.0037	0.42	56	Dense	Buoyant [d]
						30[c]	13	12	0.0016	0.0015	0.42	55	Buoyant [d]	Buoyant [d]
7664-39-3	Hydrofluoric acid	20.01	0.016	20	ERPG-2	70	124	107	0.011	0.010	0.39	61	Buoyant	Buoyant
						50	16	15	0.0014	0.0013	0.41	58	Buoyant	Buoyant
7697-37-2	Nitric acid	63.01	0.026	10	EHS-LOC (IDLH)	90	25	22	0.0046	0.0040	0.33	71	Dense	Buoyant [d]
						85	17	16	0.0032	0.0029	0.33	70	Dense	Buoyant [d]
						80	10.2	10	0.0019	0.0018	0.33	70	Dense	Buoyant [d]
8014-95-7	Oleum - based on SO_3	80.06 (SO_3)	0.010	3	ERPG-2	30 (SO_3)	3.5 (SO_3)	3.4 (SO_3)	0.0008	0.0007	0.25	93	Buoyant [d]	Buoyant [d]

Notes:

[a] Toxic endpoints are specified in the Appendix A to 40 CFR part 68 in units of mg/L. See Notes to Exhibit B-1 or B-2 for converting to other units.

[b] "Buoyant" in the Reference Table column refers to the tables for neutrally buoyant gases and vapors; "Dense" refers to the tables for dense gases and vapors. See Appendix D, Section D.4.4, for more information on the choice of reference tables.

[c] Hydrochloric acid in concentrations below 37 percent is not regulated.

[d] Use dense gas table if substance is at an elevated temperature.

Exhibit B-4
Temperature Correction Factors for Liquids Evaporating from Pools at Temperatures Between 25 ºC and 50 ºC (77 ºF and 122 ºF)

CAS Number	Chemical Name	Boiling Point (ºC)	Temperature Correction Factor (TCF)				
			30 ºC (86 ºF)	35 ºC (95 ºF)	40 ºC (104 ºF)	45 ºC (113 ºF)	50 ºC (122 ºF)
107-02-8	Acrolein	52.69	1.2	1.4	1.7	2.0	2.3
107-13-1	Acrylonitrile	77.35	1.2	1.5	1.8	2.1	2.5
814-68-6	Acrylyl chloride	75.00	ND	ND	ND	ND	ND
107-18-6	Allyl alcohol	97.08	1.3	1.7	2.2	2.9	3.6
107-11-9	Allylamine	53.30	1.2	1.5	1.8	2.1	2.5
7784-34-1	Arsenous trichloride	130.06	ND	ND	ND	ND	ND
353-42-4	Boron trifluoride compound with methyl ether (1:1)	126.85	ND	ND	ND	ND	ND
7726-95-6	Bromine	58.75	1.2	1.5	1.7	2.1	2.5
75-15-0	Carbon disulfide	46.22	1.2	1.4	1.6	1.9	LFB
67-66-3	Chloroform	61.18	1.2	1.5	1.8	2.1	2.5
542-88-1	Chloromethyl ether	104.85	1.3	1.6	2.0	2.5	3.1
107-30-2	Chloromethyl methyl ether	59.50	1.2	1.5	1.8	2.1	2.5
4170-30-3	Crotonaldehyde	104.10	1.3	1.6	2.0	2.5	3.1
123-73-9	Crotonaldehyde, (E)-	102.22	1.3	1.6	2.0	2.5	3.1
108-91-8	Cyclohexylamine	134.50	1.3	1.7	2.1	2.7	3.4
75-78-5	Dimethyldichlorosilane	70.20	1.2	1.5	1.8	2.1	2.5
57-14-7	1,1-Dimethylhydrazine	63.90	ND	ND	ND	ND	ND
106-89-8	Epichlorohydrin	118.50	1.3	1.7	2.1	2.7	3.4
107-15-3	Ethylenediamine	36.26	1.3	1.8	LFB	LFB	LFB
151-56-4	Ethyleneimine	55.85	1.2	1.5	1.8	2.2	2.7
110-00-9	Furan	31.35	1.2	LFB	LFB	LFB	LFB
302-01-2	Hydrazine	113.50	1.3	1.7	2.2	2.9	3.6
13463-40-6	Iron, pentacarbonyl-	102.65	ND	ND	ND	ND	ND
78-82-0	Isobutyronitrile	103.61	1.3	1.6	2.0	2.5	3.1
108-23-6	Isopropyl chloroformate	104.60	ND	ND	ND	ND	ND
126-98-7	Methacrylonitrile	90.30	1.2	1.5	1.8	2.2	2.6
79-22-1	Methyl chloroformate	70.85	1.3	1.6	1.9	2.4	2.9
60-34-4	Methyl hydrazine	87.50	ND	ND	ND	ND	ND
624-83-9	Methyl isocyanate	38.85	1.2	1.4	LFB	LFB	LFB
556-64-9	Methyl thiocyanate	130.00	ND	ND	ND	ND	ND
75-79-6	Methyltrichlorosilane	66.40	1.2	1.4	1.7	2.0	2.4

Exhibit B-4 (continued)

CAS Number	Chemical Name	Boiling Point (°C)	Temperature Correction Factor (TCF)				
			30 °C (86 °F)	35 °C (95 °F)	40 °C (104 °F)	45 °C (113 °F)	50 °C (122 °F)
13463-39-3	Nickel carbonyl	42.85	ND	ND	ND	ND	ND
7697-37-2	Nitric acid	83.00	1.3	1.6	2.0	2.5	3.1
79-21-0	Peracetic acid	109.85	1.3	1.8	2.3	3.0	3.8
594-42-3	Perchloromethylmercaptan	147.00	ND	ND	ND	ND	ND
10025-87-3	Phosphorus oxychloride	105.50	1.3	1.6	1.9	2.4	2.9
7719-12-2	Phosphorus trichloride	76.10	1.2	1.5	1.8	2.1	2.5
110-89-4	Piperidine	106.40	1.3	1.6	2.0	2.4	3.0
107-12-0	Propionitrile	97.35	1.3	1.6	1.9	2.3	2.8
109-61-5	Propyl chloroformate	112.40	ND	ND	ND	ND	ND
75-55-8	Propyleneimine	60.85	1.2	1.5	1.8	2.1	2.5
75-56-9	Propylene oxide	33.90	1.2	LFB	LFB	LFB	LFB
7446-11-9	Sulfur trioxide	44.75	1.3	1.7	LFB	LFB	LFB
75-74-1	Tetramethyllead	110.00	ND	ND	ND	ND	ND
509-14-8	Tetranitromethane	125.70	1.3	1.7	2.2	2.8	3.5
7550-45-0	Titanium tetrachloride	135.85	1.3	1.6	2.0	2.6	3.2
584-84-9	Toluene 2,4-diisocyanate	251.00	1.6	2.4	3.6	5.3	7.7
91-08-7	Toluene 2,6-diisocyanate	244.85	ND	ND	ND	ND	ND
26471-62-5	Toluene diisocyanate (unspecified isomer)	250.00	1.6	2.4	3.6	5.3	7.7
75-77-4	Trimethylchlorosilane	57.60	1.2	1.4	1.7	2.0	2.3
108-05-4	Vinyl acetate monomer	72.50	1.2	1.5	1.9	2.3	2.7

Notes:

ND: No data available.
LFB: Chemical above boiling point at this temperature; use LFB for analysis.

B.2 Mixtures Containing Toxic Liquids

In case of a spill of a liquid mixture containing a regulated toxic substance (with the exception of common water solutions, discussed in Section 3.3 in the text), the area of the pool formed by the entire liquid spill is determined as described in Section 3.2.2 or 3.2.3. For the area determination, if the density of the mixture is unknown, the density of the regulated substance in the mixture may be assumed as the density of the entire mixture.

If the partial vapor pressure of the regulated substance in the mixture is known, that vapor pressure may be used to derive a release rate using the equations in Section 3.2. If the partial vapor pressure of the regulated toxic substance in the mixture is unknown, it may be estimated from the vapor pressure of the pure substance (listed in Exhibit B-2, Appendix B) and the concentration in the mixture, if you assume the mixture is an ideal solution, where an ideal solution is one in which there is complete uniformity of cohesive forces. This method may overestimate or underestimate the partial pressure for a regulated substance that interacts with the other components of a mixture or solution. For example, water solutions are generally not ideal. This method is likely to overestimate the partial pressure of regulated substances in water solution if there is hydrogen bonding in the solution (e.g., solutions of acids or alcohols in water).

To estimate partial pressure for a regulated substance in a mixture or solution, use the following steps, based on Raoult's Law for ideal solutions:

- Determine the mole fraction of the regulated substance in the mixture.

  -- The mole fraction of the regulated substance in the mixture is the number of moles of the regulated substance in the mixture divided by the total number of moles of all substances in the mixture.

  -- If the molar concentration (moles per liter) of each component of the mixture is known, the mole fraction may be determined as follows:

$$X_r = \frac{M_r \times V_t}{\sum_{i=1}^{n} (M_i \times V_t)} \qquad \textbf{(B-1)}$$

or (canceling out V_t):

$$X_r = \frac{M_r}{\sum_{i=1}^{n} M_i} \qquad \textbf{(B-2)}$$

where: X_r = Mole fraction of regulated substance in mixture (unitless)
M_r = Molar concentration of regulated substance in mixture (moles per liter)
V_t = Total volume of mixture (liters)
n = Number of components of mixture
M_i = Molar concentration of each component of mixture (moles per liter)

For a mixture with three components, this would correspond to:

$$X_r = \frac{M_r}{M_r + M_2 + M_3} \quad \textbf{(B-3)}$$

where: X_r = Mole fraction of regulated substance in mixture (unitless)
M_r = Molar concentration of regulated substance (first component) in mixture (moles per liter)
M_2 = Molar concentration of second component of mixture (moles per liter)
M_3 = Molar concentration of any other components of mixture (moles per liter)

-- If the weight of each of the components of the mixture is known, the mole fraction of the regulated substance in the mixture may be calculated as follows:

$$X_r = \frac{\left(\frac{W_r}{MW_r}\right)}{\sum_{i=1}^{n}\left(\frac{W_i}{MW_i}\right)} \quad \textbf{(B-4)}$$

where: X_r = Mole fraction of the regulated substance
W_r = Weight of the regulated substance
MW_r = Molecular weight of the regulated substance
n = Number of components of the mixture
W_i = Weight of each component of the mixture
MW_i = Molecular weight of each component of the mixture

(Note: Weights can be in any consistent units.)

For a mixture with three components, this corresponds to:

$$X_r = \frac{\left(\frac{W_r}{MW_r}\right)}{\left(\frac{W_r}{MW_r}\right) + \left(\frac{W_2}{MW_2}\right) + \left(\frac{W_3}{MW_3}\right)} \quad \textbf{(B-5)}$$

where: X_r = Mole fraction of the regulated substance
W_r = Weight of the regulated substance (first component of the mixture)
MW_r = Molecular weight of the regulated substance
W_2 = Weight of the second component of the mixture
MW_2 = Molecular weight of the second component of the mixture
W_3 = Weight of the third component of the mixture
MW_3 = Molecular weight of the third component of the mixture

(Note: Weights can be in any consistent units.)

- Estimate the partial vapor pressure of the regulated substance in the mixture as follows:

$$VP_m = X_r \times VP_p \qquad \textbf{(B-6)}$$

where: VP_m = Partial vapor pressure of the regulated substance in the mixture (millimeters of mercury (mm Hg))
X_r = Mole fraction of the regulated substance (unitless)
VP_p = Vapor pressure of the regulated substance in pure form at the same temperature as the mixture (mm Hg) (vapor pressure at 25 °C is given in Exhibit B-1, Appendix B)

The evaporation rate for the regulated substance in the mixture is determined as for pure substances, with VP_m as the vapor pressure. If the mixture contains more than one regulated toxic substance, carry out the analysis individually for each of the regulated components. The release rate equation is:

$$QR = \frac{0.0035 \times U^{0.78} \times MW^{2/3} \times A \times VP}{T} \qquad \textbf{(B-7)}$$

where: QR = Evaporation rate (pounds per minute)
U = Wind speed (meters per second)
MW = Molecular weight (given in Exhibit B-2, Appendix B)
A = Surface area of pool formed by the entire quantity of the mixture (square feet) (determined as described in 3.2.2)
VP = Vapor pressure (mm Hg) (VP_m from Equation B-4 above)
T = Temperature (Kelvin (K); temperature in °C plus 273, or 298 for 25 °C)

See Appendix D, Section D.2.1 for more discussion of the evaporation rate equation. Equation B-7 is derived from Equation D-1.

Worst-case consequence distances to the toxic endpoint may be estimated from the release rate using the tables and instructions presented in Chapter 4.